

Nonextensive thermodynamics of the two-site Hubbard model: Canonical ensembles

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Abstract

Canonical ensembles consisting of M -unit *Hubbard dimers* have been studied within the nonextensive statistics (NES). The temperature dependences of the energy, entropy, specific heat and susceptibility have been calculated for the number of dimers, $M = 1, 2, 3$ and ∞ . We have assumed the relation between the entropic index q and the cluster size N given by $q = 1 + 2/N$ ($N = 2M$ for M dimers), which was previously derived by several methods. For relating the physical temperature T to the Lagrange multiplier β , two methods have been adopted: $T = 1/k_B\beta$ in the method A [Tsallis *et al.* Physica A **261**, 534 (1998)], and $T = c_q/k_B\beta$ in the method B [Abe *et al.* Phys. Lett. A **281**, 126 (2001)], where k_B denotes the Boltzmann constant, $c_q = \sum_i p_i^q$, and p_i the probability distribution of the i th state. The susceptibility and specific heat of spin dimers (*Heisenberg dimers*) described by the Heisenberg model have been discussed also by using the NES with the methods A and B. A comparison between the two methods suggests that the method B may be more reasonable than the method A for nonextensive systems.

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I. INTRODUCTION

In the last several years, much study has been made with the use of nonextensive statistics (NES) which was initiated by Tsallis [1–3]. When the physical quantity Q of a system consisting of N particles is expressed by $Q \propto N^\gamma$, it is called intensive for $\gamma = 0$, extensive for $\gamma = 1$, and nonextensive for $\gamma \neq 1$ and $\gamma \neq 0$. For example, in a spatially homogenous d -dimensional classical gas with the attractive interaction decaying as $r^{-\alpha}$, we get $\gamma = 2 - \alpha/d$ for $0 \leq \alpha/d < 1$ (nonextensive) and $\gamma = 1$ for $\alpha/d > 1$ (extensive) [3]. The nonextensivity is generally realized when the range of interactions is long enough compared to the linear size of the system. Then small-scale systems may be nonextensive even when the interaction is not long-ranged one.

Tsallis has proposed the NES entropy given by [1]

$$S_q = k_B \left(\frac{\sum_i p_i^q - 1}{1 - q} \right), \quad (1)$$

where k_B is the Boltzman constant, q the entropic index, and p_i the probability density of the i th state. Note that the entropy of BGS is obtained from Eq. (1) in the limit of $q = 1$. The quantity $|q - 1|$ expresses the measure of the nonextensivity. The NES has been successfully applied to a wide range of nonextensive systems including physics, chemistry, mathematics, astronomy, geophysics, biology, medicine, economics, engineering, linguistics, and others [4].

In our previous papers [5, 6], we have applied the NES to *Hubbard dimers* described by the two-site Hubbard model. The Hubbard model is one of the most important models in solid-state physics (for a recent review, see Ref. [7]). The Hubbard model consists of the tight-binding term expressing electron hoppings and the short-range interaction term between two electrons with opposite spins. The Hubbard model provides us with good qualitative description for many interesting phenomena such as magnetism, electron correlation, and superconductivity. In particular, the Hubbard model has been widely employed for a study on transition-metal magnetism. Thermodynamical properties of grand-canonical ensembles of a single Hubbard dimer have been calculated within the NES [5]. It has been shown that specific heat and susceptibility calculated by the NES may be significantly different from those calculated by the Boltzman-Gibbs statistics (BGS) when the entropic index q departs from unity, the NES with $q = 1$ reducing to the BGS. It is interesting to compare the calculated results with experimental data. However, experimental data for a

single dimer as adopted in Ref. [5], is not available in actual experiments. Usually experiments on nanosystems are performed on samples which include many clusters consisting of, for example, multiples dimers (for reviews, see Refs. 8-10). Iron $S = 5/2$ dimers (Fe2) in $[\text{Fe}(\text{OMe})(\text{dbm})_2]_2$ [11] have the nonmagnetic, singlet ground state and their thermodynamical property has been analyzed with the use of the Heisenberg model [12]-[14]. Similar analysis has been made for transition-metal dimers of V2 [15], Cr2 [16], Co2 [17], Ni2 [18] and Cu2 [19]. Some charge-transfer salts like tetracyanoquinodimethan (TCNQ) with dimerized structures, have been analyzed by using the two-site Hubbard model within the BGS [20]. Their susceptibility and specific heat were studied by taking into account the inter-dimer hopping, whose effect is negligibly small [20]. Such procedure may be justified within the BGS where the specific heat and susceptibility are treated as the extensive quantities: macroscopic measurements are expected to reflect the property of a constituting dimer. This is, however, not the case in the NES.

The purpose of the present paper is two folds.

(1) It is interesting and indispensable to investigate how thermodynamical properties may change when the size of a given cluster is varied within the NES. It has been shown by several methods that the entropic q of a nanosystem consisting of independent N particles is given by [21]-[23]

$$q = 1 + \frac{2}{N}. \quad (2)$$

Bearing in mind a magnetic cluster containing M transition-metal dimers, we have employed the Hubbard model to perform NES calculations for various M , assuming the relation given by

$$q = 1 + \frac{1}{M}, \quad (3)$$

which is derived from Eq. (2) with $N = 2M$ for M dimers. We have adopted $1.0 \leq q \leq 2.0$ for $1 \leq M < \infty$ in this paper, preliminary results of the M dependence of thermodynamical quantities of clusters having been reported in Ref. [6].

(2) It is not clear in the current NES how to relate the physical temperature T to the Lagrange multiplier β [5]. The following two methods have been so far proposed:

$$T = \frac{1}{k_B \beta}, \quad (\text{method A}) \quad (4)$$

$$= \frac{c_q}{k_B \beta}, \quad (\text{method B}) \quad (5)$$

where $c_q = \sum_i p_i^q$ [2]. The method A proposed in Ref. [2] is the same as the BGS. The method B is introduced so as to satisfy the *zeroth* law of thermodynamical principles and the generalized Legendre transformations [24]. It has been demonstrated that the negative specific heat of a classical gas model which is realized in the method A [25], is remedied in the method B [24]. The specific heat and susceptibility calculated by the two methods A and B are qualitatively similar, but quantitatively different: the nonextensivity calculated by the method A is generally more significant than that calculated by the method B [5, 6]. In particular, the Curie constant of the Hubbard model in the limit of vanishing couplings calculated by the method A becomes spuriously large [36] while that calculated by the method B is reasonable [5]. This is consistent with the result for localized free spins [5]. In order to get more insight to the unsettled issue on the $T - \beta$ relation, we have again made calculations with the use of methods A and B, by changing M , which is supplementary to Ref. [5].

The paper is organized as follows. After briefly reviewing the NES for the quantum system, we have derived, in Sec. 2, expressions for the specific heat and susceptibility of canonical ensembles of a cluster including dimers both in the BGS and NES, their expressions for grand-canonical ensembles having been given in Ref. [5]. In Sec. 3 numerical calculations of thermodynamical quantities are reported for various values of q and M . The final Sec. 4 is devoted to discussion and conclusion. In the Appendix, the NES has been applied to a cluster of *Heisenberg dimers*.

II. NONEXTENSIVE STATISTICS OF HUBBARD DIMERS

A. Entropy and energy

We have adopted nanoclusters including independent M Hubbard dimers with negligible interdimer interactions, each dimer being described by the two-site Hubbard model. The

total Hamiltonian is given by

$$H = \sum_{\ell=1}^M H_{\ell}^{(d)}, \quad (6)$$

$$H_{\ell}^{(d)} = -t \sum_{\sigma} (a_{1\sigma}^{\dagger} a_{2\sigma} + a_{2\sigma}^{\dagger} a_{1\sigma}) + U \sum_{j=1}^2 n_{j\uparrow} n_{j\downarrow} - \mu_B B \sum_{j=1}^2 (n_{j\uparrow} - n_{j\downarrow}), \quad (1, 2 \in \ell) \quad (7)$$

where $H_{\ell}^{(d)}$ denotes the Hamiltonian for the ℓ th dimer, $n_{j\sigma} = a_{j\sigma}^{\dagger} a_{j\sigma}$, $a_{j\sigma}$ expresses the annihilation operator of an electron with spin σ on a site j ($\in \ell$), t the hopping integral, U the intraatomic interaction, μ_B the Bohr magneton and B an applied magnetic field. Six eigenvalues of $H_{\ell}^{(d)}$ are given by

$$\epsilon_i = 0, 2\mu_B B, -2\mu_B B, U, \frac{U}{2} + \Delta, \frac{U}{2} - \Delta, \quad \text{for } i = 1 - 6 \quad (8)$$

where $\Delta = \sqrt{U^2/4 + 4t^2}$ [20][26]. The number of eigenstates of the total Hamiltonian H is 6^M .

First we employ the BGS, in which the canonical partition function for H is given by [20][26]

$$Z_{BG} = \text{Tr} \exp(-\beta H), \quad (9)$$

$$= \sum_{i_1=1}^6 \cdots \sum_{i_M=1}^6 \exp[-\beta(\epsilon_{i_1} + \cdots + \epsilon_{i_M})], \quad (10)$$

$$= [Z_{BG}^{(d)}]^M, \quad (11)$$

$$Z_{BG}^{(d)} = 1 + 2 \cosh(2\beta\mu_B B) + e^{-\beta U} + 2 e^{-\beta U/2} \cosh(\beta\Delta), \quad (12)$$

where $\beta = 1/k_B T$, Tr denotes the trace and $Z_{BG}^{(d)}$ the partition function for a single dimer. By using the standard method in the BGS, we can obtain various thermodynamical quantities of the system [20, 26, 27]. Because of the product expression given by Eq. (11), the energy and entropy are proportional to M : $E_{BG} = M E_{BG}^{(d)}$ and $S_{BG} = M S_{BG}^{(d)}$ where $E_{BG}^{(d)}$ and $S_{BG}^{(d)}$ are for a single dimer. This is not the case in the NES as will be discussed below.

The entropy S_q in the Tsallis NES is defined by [1, 2]

$$S_q = k_B \left(\frac{\text{Tr}(\rho_q^q) - 1}{1 - q} \right). \quad (13)$$

Here ρ_q stands for the generalized canonical density matrix, whose explicit form will be determined shortly [Eq. (16)]. We impose the two constraints given by

$$\text{Tr}(\rho_q) = 1, \quad (14)$$

$$\frac{\text{Tr}(\rho_q^q H)}{\text{Tr}(\rho_q^q)} \equiv \langle H \rangle_q = E_q, \quad (15)$$

where the normalized formalism is adopted [2]. The variational condition for the entropy with the two constraints given by Eqs. (14) and (15) yields

$$\rho_q = \frac{1}{X_q} \exp_q \left[- \left(\frac{\beta}{c_q} \right) (H - E_q) \right], \quad (16)$$

with

$$X_q = \text{Tr} \left(\exp_q \left[- \left(\frac{\beta}{c_q} \right) (H - E_q) \right] \right), \quad (17)$$

$$c_q = \text{Tr}(\rho_q^q) = X_q^{1-q}, \quad (18)$$

where $\exp_q[x]$ expresses the q -exponential function defined by

$$\begin{aligned} \exp_q[x] &= [1 + (1-q)x]^{\frac{1}{1-q}}, & \text{for } (1-q)x > 0 \\ &= 0, & \text{otherwise} \end{aligned} \quad (19)$$

and β is a Lagrange multiplier:

$$\beta = \frac{\partial S_q}{\partial E_q}. \quad (20)$$

The trace in Eq. (17) or (18) is performed over the 6^M eigenvalues, for example, as

$$\begin{aligned} X_q &= \sum_{i_1=1}^6 \cdots \sum_{i_M=1}^6 \left(\exp_q \left[- \left(\frac{\beta}{c_q} \right) (\epsilon_{i_1} + \cdots + \epsilon_{i_M} - E_q) \right] \right), \\ &\equiv \sum_i \left(\exp_q \left[- \left(\frac{\beta}{c_q} \right) (\epsilon_i - E_q) \right] \right), \end{aligned} \quad (21)$$

where the following conventions are adopted:

$$i = (i_1, \cdots, i_M), \quad (22)$$

$$\sum_i = \sum_{i_1=1}^6 \cdots \sum_{i_M=1}^6, \quad (23)$$

$$\epsilon_i = \epsilon_{i_1} + \cdots + \epsilon_{i_M}. \quad (24)$$

It is noted that in the limit of $q = 1$, Eq. (17) reduces to

$$X_1 = Z_{BG} \exp[\beta E_1] = [Z_{BG}^{(d)} \exp(\beta E_{BG}^{(d)})]^M. \quad (25)$$

For $q \neq 1$, however, X_q cannot be expressed as a product form because of the property of the q -exponential function:

$$\exp_q(x+y) \neq \exp_q(x) \exp_q(y) \quad \text{for } q \neq 1 \quad (26)$$

It is necessary to point out that E_q in Eq. (15) includes X_q which is expressed by E_q in Eq. (17). Then E_q and X_q have to be determined self-consistently by Eqs. (15)-(19) with Eq. (4) or (5) for a given temperature T . The calculation of thermodynamical quantities in the NES generally becomes more difficult than that in BGS.

B. Specific heat

The specific heat in the NES is given by [5, 6]

$$C_q = \left(\frac{d\beta}{dT} \right) \left(\frac{dE_q}{d\beta} \right). \quad (27)$$

Because E_q and X_q are determined by Eqs. (15)-(19), we get simultaneous equations for $dE_q/d\beta$ and $dX_q/d\beta$, given by

$$\frac{dE_q}{d\beta} = a_{11} \left(\frac{dE_q}{d\beta} \right) + a_{12} \left(\frac{dX_q}{d\beta} \right) + b_1, \quad (28)$$

$$\frac{dX_q}{d\beta} = a_{21} \left(\frac{dE_q}{d\beta} \right) + a_{22} \left(\frac{dX_q}{d\beta} \right), \quad (29)$$

with

$$a_{11} = q\beta X_q^{q-2} \sum_i w_i^{2q-1} \epsilon_i, \quad (30)$$

$$a_{12} = -X_q^{-1} E_q - \beta q(q-1) X_q^{q-3} \sum_i w_i^{2q-1} \epsilon_i (\epsilon_i - E_q), \quad (31)$$

$$a_{21} = \beta X_q^q, \quad (32)$$

$$a_{22} = 0, \quad (33)$$

$$b_1 = -q X_q^{q-2} \sum_i w_i^{2q-1} \epsilon_i (\epsilon_i - E_q), \quad (34)$$

$$\begin{aligned} w_i &= \langle i | \exp_q \left[- \left(\frac{\beta}{c_q} \right) (H - E_q) \right] | i \rangle, \\ &= \left[1 - (1-q) \left(\frac{\beta}{c_q} \right) (\epsilon_i - E_q) \right]^{\frac{1}{1-q}}, \end{aligned} \quad (35)$$

$$X_q = \sum_i w_i. \quad (36)$$

The specific heat is then given by

$$C_q = \left(\frac{d\beta}{dT} \right) \left(\frac{b_1}{1 - a_{11} - a_{12}a_{21}} \right). \quad (37)$$

with

$$\frac{\partial\beta}{\partial T} = -\beta^2, \quad (\text{method A}) \quad (38)$$

$$= - \left(\frac{\beta^2}{X_q^{1-q} - \beta(1-q)X_q^{-q}(dX_q/d\beta)} \right), \quad (\text{method B}) \quad (39)$$

In the limit of $q \rightarrow 1$, Eqs. (27)-(39) yield the specific heat in the BGS, given by [5]

$$C_{BG} = \frac{dE_{BG}}{dT} = k_B \beta^2 (\langle \epsilon_i^2 \rangle_1 - \langle \epsilon_i \rangle_1^2), \quad (40)$$

where $\langle \cdot \rangle_1$ is defined by Eq. (15).

C. Magnetization

We discuss the field-dependent magnetization, which is given in the BGS, by

$$m_{BG} = -\frac{\partial F_{BG}}{\partial B} = \langle \mu_i \rangle_1, \quad (41)$$

$$= \frac{4\mu_B \sinh(2\beta B)}{Z_{BG}} \quad (42)$$

where $\mu_i = -\partial\epsilon_i/\partial B$, Z_{BG} and $\langle \cdot \rangle_1$ are given by Eqs. (9) and (15), respectively.

In the NES, the magnetization m_q is given by

$$m_q = -\frac{\partial E_q}{\partial B} + (k_B \beta)^{-1} \frac{\partial S_q}{\partial B}, \quad (43)$$

$$= -\frac{\partial E_q}{\partial B} + \beta^{-1} X_q^{-q} \frac{\partial X_q}{\partial B} \quad (44)$$

By using Eqs. (15)-(19), we get the simultaneous equations for $\partial E_q/\partial B$ and $\partial X_q/\partial B$ given by

$$\frac{\partial E_q}{\partial B} = a_{11} \left(\frac{\partial E_q}{\partial B} \right) + a_{12} \left(\frac{\partial X_q}{\partial B} \right) + d_1, \quad (45)$$

$$\frac{\partial X_q}{\partial B} = a_{21} \left(\frac{\partial E_q}{\partial B} \right) + a_{22} \left(\frac{\partial X_q}{\partial B} \right) + d_2, \quad (46)$$

with

$$d_1 = -X_q^{-1} \sum_i w_i^q \mu_i + \beta q X_q^{q-2} \sum_i w_i^{2q-1} \epsilon_i \mu_i, \quad (47)$$

$$d_2 = \beta X_q^{q-1} \sum_i w_i^q \mu_i, \quad (48)$$

where a_{ij} ($i, j = 1, 2$) are given by Eqs. (30)-(33). We obtain m_q given by

$$m_q = \left(\frac{-c_{12} + \beta^{-1} X_q^{-q} (1 - c_{11})}{1 - c_{11} - c_{12} c_{21}} \right) d_2, \quad (49)$$

$$= X_q^{-1} \sum_i w_i^q \mu_i = \langle \mu_i \rangle_q. \quad (50)$$

In the limit of $q \rightarrow 1$, Eqs. (47) and (48) reduce to

$$d_1 = -\langle \mu_i \rangle_1 + \beta \langle \epsilon_i \mu_i \rangle_1, \quad (51)$$

$$d_2 = \beta X_1 \langle \mu_i \rangle_1, \quad (52)$$

where $\langle \cdot \rangle_1$ is given by Eq. (15) with $q = 1$. By using Eq. (50), we get $m_1 = m_{BG}$, which is given by Eq. (42).

D. Susceptibility

The high-field susceptibility in the NES is given by

$$\chi_q(B) = \frac{\partial m_q}{\partial B}. \quad (53)$$

The zero-field susceptibility $\chi_q(B = 0)$ is given by [5, 6]

$$\chi_q = \chi_q(B = 0) = -E_q^{(2)} + \beta^{-1} X_q^{-q} X_q^{(2)}, \quad (54)$$

where $E_q^{(2)} = \partial^2 E_q / \partial B^2 |_{B=0}$ and $X_q^{(2)} = \partial^2 X_q / \partial B^2 |_{B=0}$. With the use of Eqs. (15)-(19), we get simultaneous equations for $E_q^{(2)}$ and $X_q^{(2)}$ given by

$$E_q^{(2)} = a_{11} E_q^{(2)} + a_{12} X_q^{(2)} + f_1, \quad (55)$$

$$X_q^{(2)} = a_{21} E_q^{(2)} + a_{22} X_q^{(2)} + f_2, \quad (56)$$

with

$$f_1 = -2 \beta q X_q^{q-2} \sum_i w_i^{2q-1} \mu_i^2, \quad (57)$$

$$f_2 = \beta^2 q X_q^{2(q-1)} \sum_i w_i^{2q-1} \mu_i^2, \quad (58)$$

where a_{ij} ($i, j = 1, 2$) are given by Eqs. (30)-(33). From Eqs. (54)-(58), we get

$$\chi_q = \frac{f_2}{a_{21}} = \beta q X_q^{q-2} \sum_i w_i^{2q-1} \mu_i^2 |_{B=0}. \quad (59)$$

In the limit of $q = 1$, Eq. (59) yields the susceptibility in BGS:

$$\chi_{BG} = \beta \langle \mu_i^2 \rangle_{B=0} > 1, \quad (60)$$

$$= \left(\frac{\mu_B^2}{k_B T} \right) \left(\frac{8}{3 + e^{-\beta U} + 2e^{-\beta U/2} \cosh(\beta \Delta)} \right). \quad (61)$$

III. CALCULATED RESULTS

A. The q dependence

We have performed numerical calculations by changing the index q or the size of a cluster M in the NES. Simultaneous equations for E_q and X_q given by Eqs. (15)-(19) have been solved by using the Newton-Raphson method with initial values of E_1 and X_1 obtained from BGS ($q = 1$). The magnetic field B in Eq. (8) is set zero in calculating the entropy, energy and specific heat. The calculated quantities are given *per dimer*.

— — — — — *Fig.1* — — — — —

First we treat the entropic index q as a free parameter for a single dimer. Figures 1(a)-1(f) show the temperature dependence of the energy E_q calculated for $B = 0$. Bold solid curves in Fig. 1(a), 1(b) and 1(c) show E_1 in the BGS calculated for $U/t = 0, 5$ and 10 , respectively. The ground-state energy at $T = 0$ is $E_1/t = -2.0, -0.70156$ and -0.38516 for $U/t = 0, 5$ and 10 , respectively. With increasing q value above unity, the gradient of E_q is much decreased in the method A, as shown in Figs. 1(a)-1(c). This trend is, however, much reduced in the method B, as Figs. 1(d)-1(f) show. This behavior is more clearly seen in the temperature dependence of the specific heat C_q , as will be discussed shortly [Figs. 3(a)-3(f)].

— — — — — *Fig.2* — — — — —

Temperature dependences of the entropy for $B = 0$ are plotted in Figs. 2(a)-2(f). Figures 2(a), 2(b) and 2(c) express S_q for $U/t = 0, 5$ and 10 , respectively, calculated by the method A, and Figs. 2(d)-2(f) those calculated by the method B. Bold curves denote the results for

the BGS, where the entropy is quickly increased at low temperature when the interaction is increased. When the q value is more increased above unity, S_q is more rapidly increased at very low temperatures and its saturation value at higher temperatures becomes smaller. This behavior is commonly realized in the results calculated by the methods A and B. A difference between the two results is ostensibly small because S_q shows a saturation at low temperatures.

— — — — — *Fig.3* — — — — —

Figures 3(a)-3(f) show the specific heat calculated for $B = 0$. C_1 in BGS for $U/t = 0$ shown by the bold solid curve in Fig. 3(a), has a peak at $k_B T/t \sim 0.65$. Figure 3(c) shows that for $U/t = 10$, this peak splits into two. A lower peak arises from low-lying collective spin-wave-like excitations while higher one from single-particle excitations [20, 27]. For intermediate $U/t = 5$ these two peaks overlap [Fig. 3(b)]. The temperature dependences of the specific heat C_q calculated with the use of the method A for $U/t = 0, 5$ and 10 are plotted in Figs. 3(a), 3(b) and 3(c), respectively. We note that when q is larger than unity, peaks become broader. Figures 3(d), 3(e) and 3(f) show the temperatures dependence of the specific heat C_q calculated by the method B for $U/t = 0, 5$ and 10 , respectively. Although general property of the q dependence of the specific heat of the method B is similar to that of the method A, the effect of the nonextensivity in the method B becomes smaller than that in the method A.

— — — — — *Fig.4* — — — — —

The BGS susceptibility for $U/t = 0$ has a peak at $k_B T/t \sim 0.65$ as Fig. 4(a) shows. With increasing U/t , the magnitude of χ_{BG} is enhanced by the interaction, and its peak position becomes lower [20, 27], as Figs. 4(b) and 4(c) show: the horizontal scale of Fig. 4(c) is enlarged compared with Figs. 4(a) and 4(b). The temperature dependences of the susceptibility χ_q calculated by the method A for $U/t = 0, 5$ and 10 are plotted in Figs. 4(a), 4(b) and 4(c), respectively. We note that as increasing q above unity, the peak in χ_q becomes broader. Figures 4(d), 4(e) and 4(f) show the temperature dependence of the susceptibility

χ_q calculated by the method B for $U/t = 0, 5$ and 10 , respectively. Again the effect of the nonextensivity in the method B becomes smaller than that in the method A.

B. The M dependence

-----Fig.5-----

In order to study how thermodynamical quantities of a cluster with Hubbard dimers depend on its size M , we have made NES calculations, assuming the q value for a given M value with the $M - q$ relation given by Eq. (3). Results for $M = \infty$ correspond to those of the BGS ($q = 1$). Figures 5(a)-5(d) show the results for non-interacting case of $U/t = 0$. The specific heat and susceptibility shown in Figs. 5(a) and 5(b), have been calculated by the method A with $q = 2.0, 1.5$, and 1.333 for $M = 1, 2$ and 3 , respectively. Figures 5(c) and 5(d) express C_q and χ_q , respectively, calculated by the method B. We note that physical quantities in a small cluster with $M \sim 1 - 3$ are rather different from those of bulk-like systems with $M = \infty$, although properties of clusters gradually approach those of bulk with increasing M .

-----Fig.6-----

Similar results for finite interaction of $U/t = 5$ are shown in Figs. 6(a)-6(d). The specific heat and susceptibility plotted in Figs. 6(a) and 6(b), respectively, have been calculated by the method A for $M = 1, 2, 3$ and ∞ . Figures 6(c) and 6(d) show C_q and χ_q , respectively, calculated by the method B for $U/t = 5$. The results for small M are very different from those for $M = \infty$. We note that the M dependences of C_q and χ_q of Hubbard dimers shown in Figs. 6(a)-6(d) are similar to those of spin dimers described by the Heisenberg model [Figs. 13(a)-13(d)], details being discussed in the Appendix A. This is not surprising because the Hubbard model with the strong coupling and the half-filled electron occupancy, reduces to the Heisenberg model with the antiferromagnetic exchange interaction.

-----Fig.7-----

We have calculated the M dependence of the maximum values of C_q^* and χ_q^* and corresponding temperatures of T_C^* and T_χ^* . Figure 7(a) shows T_C^* and T_χ^* , and Fig. 7(b) depicts C_q^* and χ_q^* , all of which are plotted against $1/M$: solid and dashed lines denote results calculated by the methods A and B, respectively. It is shown in Fig. 7(a) that with increasing $1/M$, T_χ^* calculated by the method A is much increased than that calculated by the method B. We note also that with increasing $1/M$, T_C^* of the method B is increased while that of the method A is decreased. Figure 7(b) shows that C_q^* in the method A is smaller than that in the method B, whereas χ_q^* in the method A is the same as that in the method B.

IV. DISCUSSIONS AND CONCLUSIONS

— — — — — *Fig.8* — — — — —

Although we have discussed the temperature dependence of physical quantities in the preceding section, it is worthwhile to study their magnetic-field dependence. Figures 8(a), 8(b) and 8(c) show the magnetization m_q as a function of the magnetic field B for $U/t = 0$, 1 and 10, respectively, at $k_B T/t = 1.0$ calculated by the method A: results calculated by the method B is not so different from them [Figs. 10(a)]. When q is increased above unity, the magnetization at lower fields ($h/t < 1$) is decreased whereas at higher fields ($h/t > 1$) it is much increased. This is consistent with the calculation of the susceptibility shown in Fig. 3(a)-3(c), where χ_q at $k_B T/t = 1.0$ is smaller for larger q : the susceptibility stands for the initial gradient of m_q at $B = 0$.

— — — — — *Fig.9* — — — — —

— — — — — *Fig.10* — — — — —

The field dependence of physical quantities are discussed in more details. Figure 9 shows the B dependence of the six eigenvalues of ϵ_i for $U/t = 5$ [Eq. (8)]. We note the crossing of

the eigenvalues of ϵ_3 and ϵ_6 at the critical field:

$$\mu_B B_c = \sqrt{\frac{U^2}{16} + t^2} - \frac{U}{4}, \quad (62)$$

leading to $\mu_B B_c/t = 0.351$ for $U/t = 5$. At $B = B_c$ the magnetization m_q is rapidly increased as shown in Figs. 10(a) and 10(b) for $k_B T/t = 1.0$ and 0.1 , respectively: the transition at lower temperature is more evident than at higher temperature. This level crossing also yields a peak in χ_q [Figs. 10(c) and 10(d)] and a dip in C_q [Figs. 10(e) and 10(f)]. It is interesting that the peak of χ_q for $q = 1.5$ in the NES is more significant than that in the BGS whereas that of C_q of the former is broader than that of the latter. When the temperature becomes higher, these peak structures become less evident. Similar phenomenon in the field-dependent specific heat and susceptibility have been pointed out in the Heisenberg model within the BGS [28].

Figure 10(a) and 10(b) remind us the quantum tunneling of magnetization observed in magnetic molecular clusters such as Mn4, Mn12 and Fe8 [29]. It originates from the level crossing of magnetic molecules which are parallel and anti-parallel to the easy axis when a magnetic field is applied.

The $N - q$ relation given by $q = 1 + 2/N$ [Eq. (2)] has been derived from the average of the BGS partition function of $\exp(-\beta\epsilon)$ with $\epsilon = \sum_i \epsilon_i$ over fluctuating β fields, as given by [21]-[23]

$$w(\{\epsilon_i\}) = \int_0^\infty d\beta \exp\left(-\beta \sum_{i=1}^N \epsilon_i\right) f^B(\beta) = \exp_q \left[-\beta_0 \sum_{i=1}^N \epsilon_i \right], \quad (63)$$

with

$$f^B(\beta) = \frac{1}{\Gamma\left(\frac{N}{2}\right)} \left(\frac{N}{2\beta_0}\right)^{\frac{N}{2}} \beta^{\frac{N}{2}-1} \exp\left(-\frac{N\beta}{2\beta_0}\right), \quad (64)$$

$$\beta_0 = \langle \beta \rangle, \quad (65)$$

$$\frac{2}{N} = \frac{\langle \beta^2 \rangle - \langle \beta \rangle^2}{\langle \beta \rangle^2}. \quad (66)$$

Here $\langle Q \rangle$ stands for the expectation value of Q averaged over the Γ (or χ^2) distribution function $f^B(\beta)$, β_0 the average of the fluctuating β and $2/N$ its variance. The Γ distribution is emerging from the sum of squares of N Gaussian random variables. Alternatively, by using the large-deviation approximation, Touchette [30] has obtained the distribution function $f^T(\beta)$, in place of $f^B(\beta)$, given by

$$f^T(\beta) = \frac{\beta_0}{\Gamma\left(\frac{N}{2}\right)} \left(\frac{N\beta_0}{2}\right)^{\frac{N}{2}} \beta^{-\frac{N}{2}-2} \exp\left(-\frac{N\beta_0}{2\beta}\right). \quad (67)$$

Figure 11 shows the f^B - and f^T -distribution functions for various N values. For $N \rightarrow \infty$, both reduce to the delta-function densities, and for a large $N = 100$, both distribution functions lead to similar results. For a small $N (< 10)$, however, there is a clear difference between the two distribution functions. We note that a change of variable $\beta \rightarrow \beta^{-1}$ in f^T yields the distribution function similar to f^B . It should be noted that f^T cannot lead to the q -exponential function which plays a crucial role in the NES. For a large ϵ , f^T leads to the stretched exponential form of $w(\epsilon) \sim e^{c\sqrt{\epsilon}}$ while f^B yields the power form of $w(\epsilon) \sim \epsilon^{-\frac{1}{q-1}}$. This issue of f^B vs. f^T is related to the *superstatistics*, which is currently studied with much interest [31].

In deriving Eq. (63), we have implicitly assumed that the distance between sparsely distributed clusters is larger than ξ , the *coherence* length of the fluctuating β field over which the field β uniformly fluctuates, and that the linear size of the clusters is smaller than ξ . If the population of constituting dimers in a given cluster is sparse such that the distance between dimers is larger than ξ and a local fluctuating β_i field around a dimer i is almost independent from the local β_j field around another dimer j , Eq. (64) is replaced by

$$w(\{\epsilon_i\}) = \Pi_{i=1}^N \int_0^\infty d\beta_i \exp(-\beta_i \epsilon_i) f^B(\beta_i) = \Pi_{i=1}^N \exp_{q'}[-\beta_0 \epsilon_i], \quad (68)$$

with $q' = 3$. Actual distribution of dimers is expected to lie between the two extreme cases given by Eqs. (63) and (68) [22].

Although results calculated by the two methods A and B are qualitatively similar, there are some quantitative difference, as previously obtained in Refs. [5] and [6]. When we calculate the Curie constant Γ_q of the susceptibility defined by $\chi_q(T) = (\mu_B^2/k_B)[\Gamma_q(T)/T]$, the ratio between $\Gamma_q^{(A)}$ and $\Gamma_q^{(B)}$ calculated by the two methods, is given by

$$\frac{\Gamma_q^{(A)}}{\Gamma_q^{(B)}} = c_q, \quad (69)$$

$$= 4^{(q-1)}, \quad \text{for } T = 0 \quad (70)$$

$$= 6^{(q-1)}. \quad \text{for } T = \infty \quad (71)$$

In general, $\Gamma_q^{(B)}$ depends on t , U and T . In the limit of $t = 0$, for example, it is given by [32]

$$\Gamma_q^{(B)} = 2q, \quad \text{for } T = 0 \quad (72)$$

$$= \frac{4}{3}q. \quad \text{for } T = \infty \quad (73)$$

The result of the method A given by Eqs. (69)-(73) leads to anomalously large Curie constant compared to that of the method B. Equation (69) is consistent with the result for spin dimers described by the Heisenberg model (for details, see Appendix A) [5]. A comparison between Eqs. (35) and (63) yield the average temperature $\langle T \rangle$ given by

$$\frac{1}{k_B \langle T \rangle} \simeq \beta_o = \frac{c_q}{\beta} \quad (74)$$

which supports the method B. These results suggest that the method B is more appropriate than the method A. This is consistent with recent theoretical analyses made in [33, 34] (for related discussions, see Ref. [35]).

In summary, within the framework of the NES, thermodynamical properties have been discussed of a cluster including M dimers, each of which is described by the two-site Hubbard model. We have demonstrated that the thermodynamical properties of small-scale systems are rather different from those of bulk systems. Owing to recent progress in atomic engineering, it is possible to synthesize molecules containing relatively small numbers of magnetic atoms with the use of various methods (for reviews, see refs. 8-10). Small-size magnetic systems ranging from grains (micros), nanosystems, molecular magnets and atomic clusters, display a variety of intriguing physical properties. It is interesting to compare our theoretical prediction with experimental results for samples containing small number of transition-metal dimers of $M = 1, 2$ and 3 . Unfortunately experiments on samples with such a very small number of dimers, have not been reported. Theoretical and experimental studies on nanoclusters with changing M could clarify a link between the behavior of the low-dimensional infinite systems and nanoscale finite-size systems. The unsettled issues on $T - \beta$ and the $N - q$ relations in the current NES are expected to be resolved by future theoretical and experimental studies on nanosystems, which are expected to be one of ideal systems for a study on the NES. Our discussion in this study has been confined to the static property of nanoclusters. It would be interesting to investigate dynamics of dimers which has been discussed within the framework of the BGS.

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Appendix: NES for Heisenberg dimers

We consider a cluster containing M Heisenberg dimers, spin dimers described by the Heisenberg model ($s = 1/2$), given by

$$H = \sum_{\ell=1}^M H_{\ell}^{(d)}, \quad (\text{A1})$$

$$H_{\ell}^{(d)} = -J\mathbf{s}_1 \cdot \mathbf{s}_2 - g\mu_B B(s_{1z} + s_{2z}), \quad (1, 2 \in \ell) \quad (\text{A2})$$

where J stands for the exchange interaction, g ($=2$) the g-factor, μ_B the Bohr magneton, and B an applied magnetic field. Four eigenvalues for $H_{\ell}^{(d)}$ are given by

$$\begin{aligned} \epsilon_i &= -\frac{J}{4} - g\mu_B B m_i, & \text{with } m_1 = 1, 0, -1 \text{ for } i = 1, 2, 3 \\ &= \frac{3J}{4} - g\mu_B B m_i. & \text{with } m_4 = 0 \text{ for } i = 4 \end{aligned} \quad (\text{A3})$$

The number of eigenvalues of H becomes 4^M .

In the BGS the canonical partition function is given by

$$Z_{BG} = [Z_{BG}^{(d)}]^M, \quad (\text{A4})$$

$$Z_{BG}^{(d)} = \exp\left(\frac{\beta J}{4}\right) [1 + 2\cosh(2\beta\mu_B B)] + \exp\left(-\frac{3\beta J}{4}\right), \quad (\text{A5})$$

with which thermodynamical quantities are easily calculated. The susceptibility is, for example, given by [12, 13]

$$\chi_{BG} = M\chi_{BG}^{(d)}, \quad (\text{A6})$$

$$\chi_{BG}^{(d)} = \left(\frac{\mu_B^2}{k_B T}\right) \left(\frac{8}{3 + \exp(-J/k_B T)}\right). \quad (\text{A7})$$

The calculation of thermodynamical quantities in the NES for the Heisenberg model goes parallel to that discussed in Sec. 2 if we employ eigenvalues given by Eq. (A3). For example, by using Eq. (59), we get the zero-field susceptibility for Heisenberg dimers, given by

$$\chi_q = g^2 \mu_B^2 \left(\frac{q\beta}{c_q}\right) \frac{1}{X_q} \sum_i w_i^{2q-1} m_i^2, \quad (\text{A8})$$

where a sum \sum_i is performed over 4^M eigenvalues [see Eq. (23)]. In the case of $M = 1$ (a

single dimer), we get

$$\chi_q^{(d)} = g^2 \mu_B^2 \left(\frac{q\beta}{c_q} \right) \left(\frac{2}{X_q} \right) \left(\exp_q \left[\left(\frac{\beta}{c_q} \right) \left(\frac{J}{4} + E_q \right) \right] \right)^{2q-1}, \quad (\text{A9})$$

$$X_q = 3 \exp_q \left[\left(\frac{\beta}{c_q} \right) \left(\frac{J}{4} + E_q \right) \right] + \exp_q \left[\left(-\frac{\beta}{c_q} \right) \left(\frac{3J}{4} - E_q \right) \right], \quad (\text{A10})$$

$$E_q = \frac{1}{X_q} \left\{ \left(\frac{-3J}{4} \right) \left(\exp_q \left[\left(\frac{\beta}{c_q} \right) \left(\frac{J}{4} + E_q \right) \right] \right)^q + \left(\frac{3J}{4} \right) \left(\exp_q \left[\left(-\frac{\beta}{c_q} \right) \left(\frac{3J}{4} - E_q \right) \right] \right)^q \right\}. \quad (\text{A11})$$

In the limit of $q = 1$, Eq. (A9) reduces to $\chi_{BG}^{(d)}$ given by Eq. (A7).

The Curie constant Γ_q defined by $\chi_q = (\mu_B^2/k_B)(\Gamma_q/T)$ for $J = 0$ is given by [5]

$$\Gamma_q = 2M q 4^{M(q-1)}, \quad (\text{method A}) \quad (\text{A12})$$

$$= 2M q, \quad (\text{method B}) \quad (\text{A13})$$

which are consistent with results obtained for Hubbard dimes [5]. Equations (A12) leads to an anomalously large Curie constant, which was referred to as *dark magnetism* in Ref. [36].

— — — — — Fig.12 — — — — —

Figure 12(a) and 12(b) show the temperature dependences of the specific heat and susceptibility, respectively, of a single Heisenberg dimer ($M = 1$) for several q values for $J < 0$ (antiferromagnetic coupling) calculated by the method A (solid curves) and B (dashed curves). Figures 12(c) and 12(d) show the specific heat and susceptibility, respectively, of two spin dimers ($M = 2$) calculated with the use of 4^2 eigenvalues.

— — — — — Fig.13 — — — — —

Figures 13(a) and 13(b) show C_q and χ_q when the size M of a cluster of Heisenberg dimers is changed, with $q = 2.0, 1.5, 1.333$ and 1.25 for $M = 1, 2, 3$ and 4 , respectively, calculated by the method A: results for $q = 1$ of the BGS [corresponding to $M = \infty$ in Eq. (3)] are included for a comparison. Figs. 13(c) and 13(d) show similar results of C_q and χ_q

calculated by the method B. The M dependence of C_q and χ_q for Heisenberg dimers shown in Fig. 13(a)-13(d) is quite similar to those shown in Figs. 6(a)-6(d) for Hubbard dimers.

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FIG. 1: The temperature dependences of the energy E_q for $B = 0$ with (a) $U/t = 0$, (b) 5 and (c) 10 calculated by the method A, and those with (d) $U/t = 0$, (e) 5 and (f) 10 calculated by the method B: $q = 1.0$ (bold solid curves), 1.1 (dotted curves), 1.2 (dashed curves), 1.5 (chain curves) and 2.0 (solid curves).

FIG. 2: The temperature dependences of the entropy S_q for $B = 0$ with (a) $U/t = 0$, (b) 5 and (c) 10 calculated by the method A, and those with (d) $U/t = 0$, (e) 5 and (f) 10 calculated by the method B: $q = 1.0$ (bold solid curves), 1.1 (dotted curves), 1.2 (dashed curves), 1.5 (chain curves) and 2.0 (solid curves).

FIG. 4: The temperature dependences of the susceptibility χ_q for $B = 0$ for (a) $U/t = 0$, (b) 5 and (c) 10 calculated by the method A, and those for (d) $U/t = 0$, (e) 5 and (f) 10 calculated by the method B: $q = 1.0$ (bold solid curves), 1.1 (dotted curves), 1.2 (dashed curves), 1.5 (chain curves) and 2.0 (solid curves).

FIG. 5: The temperature dependences of (a) specific heat C_q and (b) susceptibility χ_q (per dimer) of Hubbard dimers for $U/t = 0$ calculated by the method A, and those of (c) specific heat C_q and (d) susceptibility χ_q calculated by the method B, with $M = 1$ (bold solid curves), $M = 2$ (chain curves), $M = 3$ (dashed curves) and $M = \infty$ (solid curves).

FIG. 6: The temperature dependences of (a) specific heat C_q and (b) susceptibility χ_q (per dimer) of Hubbard dimers for $U/t = 5$ calculated by the method A, and those of (c) specific heat C_q and (d) susceptibility χ_q calculated by the method B, with $M = 1$ (bold solid curves), $M = 2$ (chain curves), $M = 3$ (dashed curves) and $M = \infty$ (solid curves).

FIG. 3: The temperature dependences of the specific heat C_q for $B = 0$ with (a) $U/t = 0$, (b) 5 and (c) 10 calculated by the method A, and those with (d) $U/t = 0$, (e) 5 and (f) 10 calculated by the method B: $q = 1.0$ (bold solid curves), 1.1 (dotted curves), 1.2 (dashed curves), 1.5 (chain curves) and 2.0 (solid curves).

FIG. 7: (a) $1/M$ dependence of the temperatures of T_C^* (circles) and T_χ^* (squares) where C_q and χ_q have the maximum values, respectively. (b) $1/M$ dependence of the maximum values of C_q^* (circles) and χ_q^* (squares). Solid and dashed lines denote the results calculated by the methods A and B, respectively: T_χ^* calculated by the method A shown in (a) is divided by a factor of five.

FIG. 8: The magnetization m_q as a function of the magnetic field B for (a) $U/t = 0$, (b) 1 and (c) 10 at $k_B T/t = 1.0$: $q = 0.8$ (double-chain curves), 0.9 (chain curves), 1.0 (bold solid curves), 1.1 (dotted curves), 1.2 (dashed curves), and 1.5 (solid curves) calculated by the method A.

FIG. 9: The magnetic-field dependence of the eigenvalues ϵ_i ($i = 1 - 6$), for $U/t=5$.

FIG. 10: The magnetic-field dependence of (a) the magnetization m_q for $k_B T/t = 1.0$ and (b) $k_B T/t = 0.1$, (c) the susceptibility for $k_B T/t = 1.0$ and (d) $k_B T/t = 0.1$, (e) the specific heat χ_q for $k_B T/t = 1.0$ and (f) $k_B T/t = 0.1$, of a single Hubbard dimer ($M = 1$) for $U/t=5$, calculated by the method A (solid curves) method B in the NES (dashed curves), and in the BGS (chain curves).

FIG. 11: The distributions of $f^B(\beta)$ (solid curves) and $f^T(\beta)$ (dashed curves) as a function of β (see text).

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